SUPPLEMENTARY MATERIAL
SPINE SAMPLE HOLDER & VIAL STANDARD SPECIFICATIONS-L-R04

The specifications in this appendix are based on SPINE document version L-R04. The document has been posted on the SPINE website (http://www.spineurope.org) in revised form on the 15th November 2004.

1. Summary and design guidelines

A SPINE workshop was held in Grenoble in 2002 (see meetings page, SPINE website) to discuss how best to formulate a sample holder standard for general use. Although in the first instance, the primary goal was to obtain a European standard for use by SPINE partners and associates. The following criteria for the standard, were put in place after this workshop:

1) The design of the standard should be easily adaptable for use with robots that in 2002 were available commercially or academically and were using Hampton Research magnetic caps. At this time robots were available and/or in development from Mar research – (marcsc), Rigaku (ACTOR), Bruker Nonius (BruNo), EMBL/ESRF Grenoble, EMBL Hamburg, CNRS Grenoble (FIP), SSRL and ALS.
2) Be compatible with the hampton magnetic sample holder and vial system
3) Accept different pin types for versatile holder options
4) Identification with ECC200 DATA MATRIX codes and a human readable code
5) Improved precision for robotic handling
6) Improved stability for use with micro crystals
7) Compatible with manual use
8) Public design to allow production by multiple manufacturing companies

2. Terminology

The sample holder standard is based on the CrystalCap Magnetic™ system of Hampton research. The standard consists principally of a cap which is the support/base for the sample pin that holds the sample support (be it a nylon loop, litholoop, etc) and an associated vial. The following definitions and descriptions have been agreed:

1. **The Cap**: this is the support/base for the pin which holds the sample support magnetic crystal cap. (see Information drawing 1 reference *DM16106A)*
2. **Pin**: steel support with mounted crystal support (nylon loop or other)
3. **Sample holder**: This consists of the Cap and the Pin (see Information drawing 2, reference *DM16100*)
4. **Sample holder length**: This is defined as the distance from the base of the cap to the mounted sample. See Figure 1 (b) in main paper and Information drawing 2)
5. **Vial**: container to hold sample in Liquid nitrogen reservoir. See information drawing 3 and 4, references *DM16210*A *and DM16001A*
6. **Goniometer mount**: Magnet or electromagnet that holds the Sample holder on the goniometer, see information drawing 5, reference *DM16300*

3. Features of the Sample holder component parts

3.1 The Cap

The cap is shown for information in drawing 1 and has the following main features:

- Rounded edges (or chamfers) to avoid potential blocking during transfers.
- Recommended material: Steel anticorrosion coated or ferromagnetic stainless steel (Stainless steel 430F or equivalent).
- Minimum material quantity to reduce the freezing/melting/drying cycle when the sample holder is transferred
- Pinhole diameter and depth are not specified. This is dependent on the type of pin used. An example is given for a 18 mm Hampton "Mounted Cryoloop™" in information drawing 2.
- DATA MATRIX code protection when a sample holder is mounted on a goniometer mount: A gap is maintained between the code and the mount. The surface of contact between the cap and the Goniometer mount is the cap Base (Information drawing 4). The surface of the internal disc (Φ9.7mm) is reserved for labelling. The stability of the sample holder is improved when mounted on the Goniometer. The sample holder remains compatible with existing goniometer mounts.

3.2 Sample holder Length

The sample holder length has been fixed at 22mm to ensure compatibility with all sample changers. The length is defined from the base of the cap to the sample position. The pin should be attached with the following criteria:

- The sample holder length is **22 mm** (from base of cap to crystal or beam position)
- A fixed Sample Holder length will ensure compatibility with all sample changers
- The pin should be stably attached to the cap

3.2Vials

The vial standard as shown for information in drawing 3 has the following main features*:*

- Rounded edges (or chamfers) on the top and on the bottom of the vials to avoid potential blocking during transfers.
- A ferromagnetic disc at the bottom of the vials for "positive" vial manipulation with a magnet
- Polarity of the vial magnetic ring is specified
- Vent hole

4. Sample Holder identification:

The cap of the sample holder is identified with a 2-D data matrix code with an equivalent human readable code on the side of the cap (See Figure 1 (a). The data matrix code positioning and specification recommendations are:

1. **ECC200 DATA MATRIX** label is placed on the top of the cap. This can be either printed or engraved on the magnet footprint face (Φ 9.7 mm).
2. A human Readable code should be placed near the DATA MATRIX code and/or on the rim of the Cap.
3. The data matrix should be readable in LN2, cold and Room temperature environments.

4.1 ID encoding scheme

A **Sample Holder ID** should be composed of a string of 10 alphanumerical characters**:**

MA12BC3456.

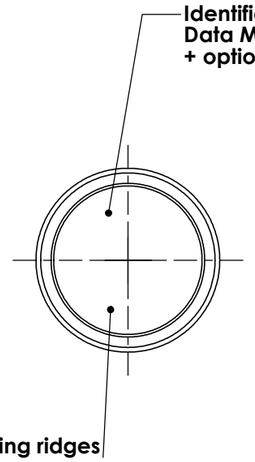
MA12BC3456.
The first letter identifies the manufacturer and ensures that different manufactures cannot produce the same ID.
Contact spine.sh.mid@spineurope.org for attribution of the Manufacturers IDs.
See Annex 1.

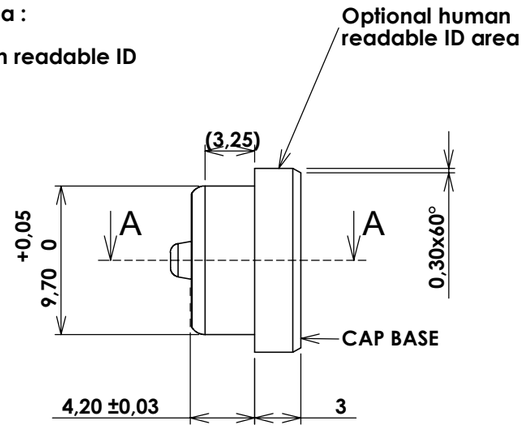
M**A12BC3456.**
The remaining 9 characters are organised for good human readability into 1 character, 2 numbers, 2 letters, followed by 4 numbers. These numbers and letters are random.

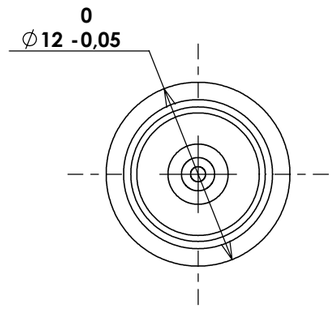
4.2 DATA MATRIX format

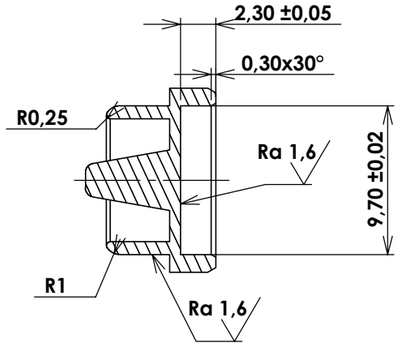
Allowed ECC200 DATA MATRIX codes are:

	Format Number	Numeric Capacity	Alphanumeric capacity	Correctable Errors/Erasures
14x14	2	16	10	5/7
16x16	3	24	16	6/9



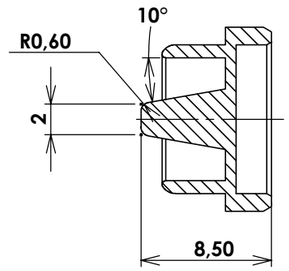






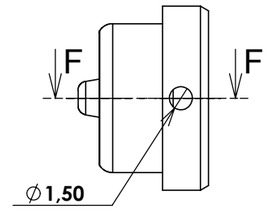
A-A

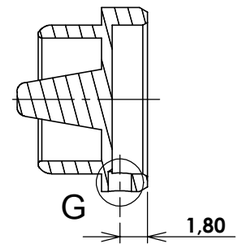
Non critical dimensions



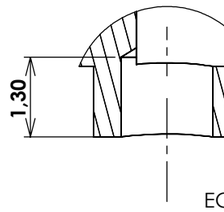
COUPE A-A

Option 1 : hole for LN2 evacuation



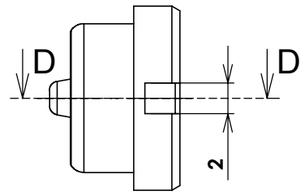


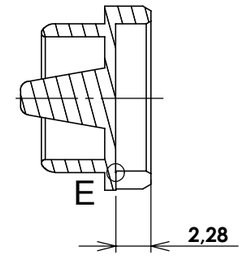
COUPE F-F



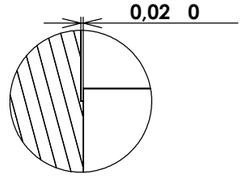
DÉTAIL G
ECHELLE 10 : 1

Option 2 : groove for LN2 evacuation



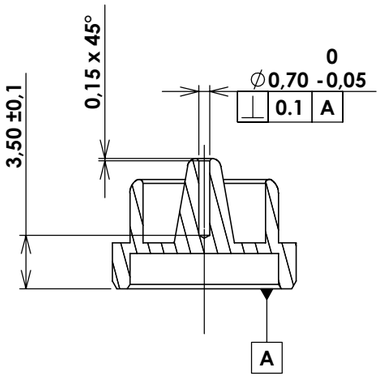


COUPE D-D

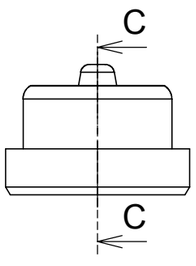


DÉTAIL E
ECHELLE 20 : 1

Example :Pin hole for 18mm Hampton pin



COUPE C-C



Drawing only for information

Notes: - Recommanded materials : 430F - DIN 1.4104 - X14 CrMoS17

c			
b			
a	18/06/2004	cotation updated, options added	
	Date	Modification	Auteur

Titre

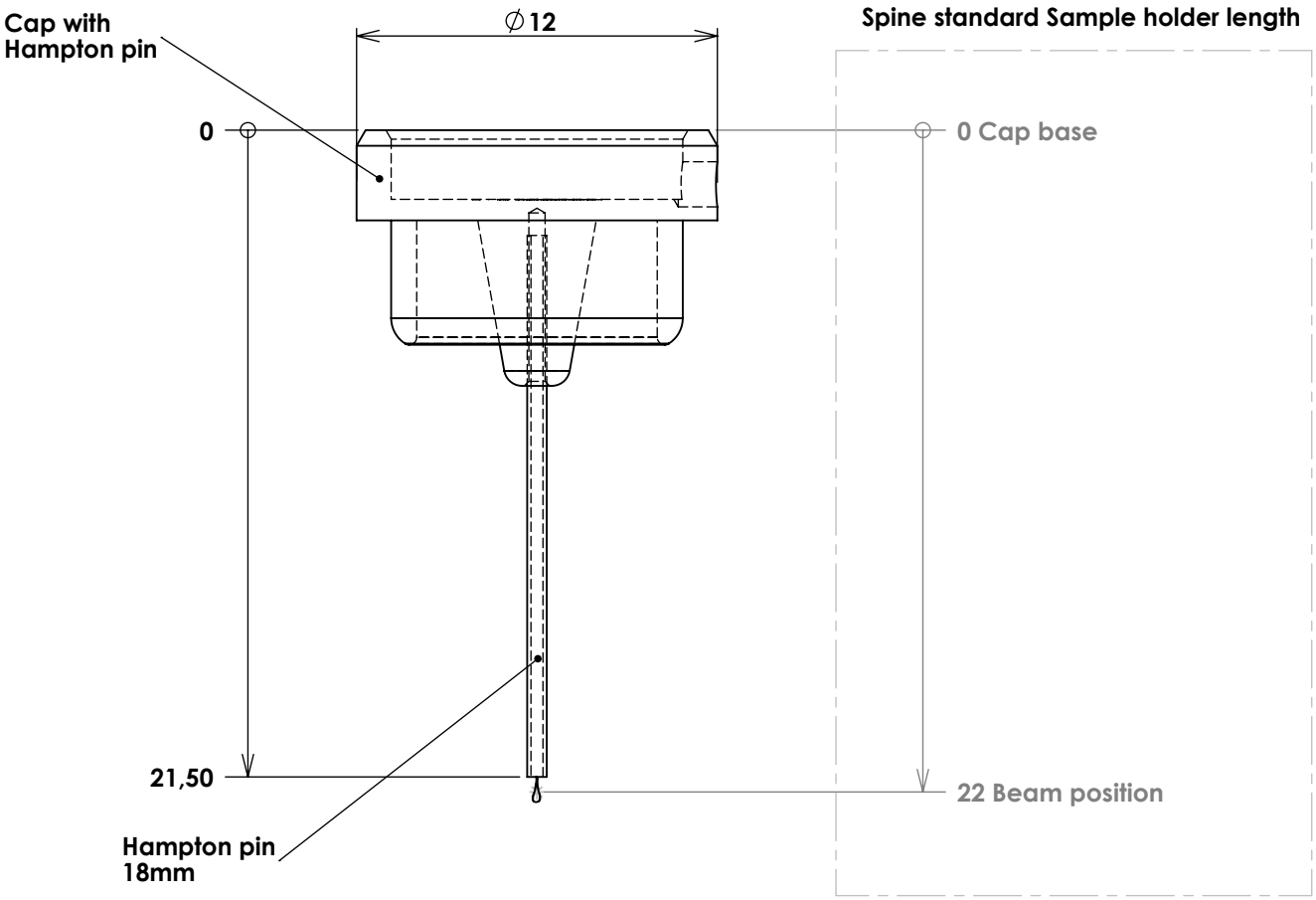
Spine Cap

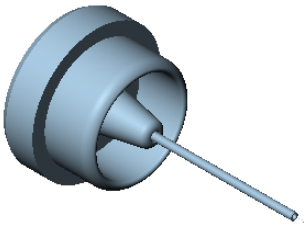
A3

Tolérances générales (sauf indications) JS13 - Ra 3,2 - angles cassés à 0,2mm

Numéro - Indice de mise à jour **DM 16106 A**	Projet : Spine - WP6	
	Sous-ensemble :	
Matière :	Remarque :	Qté : -
Dessiné : PY LANQUETIN	Date : 11-03-2003	Echelle : 2.5:1

EMBL
Antenne de Grenoble
Laboratoire Européen de Biologie Moléculaire
6, rue Jules Horowitz - 38000 Grenoble
téléphone 0 476 207 188 - fax 0 476 207 199





c			
b			
a			
	Date	Modification	Auteur

Titre

Sample holder

A4

Tolérances générales (sauf indications) JS13 - Ra 3,2 - angles cassés à 0,2mm

Numéro - Indice de mise à jour

DM 16100

Projet : SPINE + WP6

Sous-ensemble :

Matière :

Remarque :

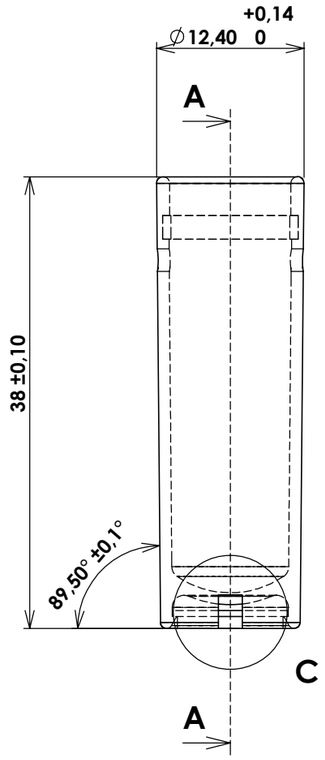
Qté : 1

Dessiné : PY LANQUETIN

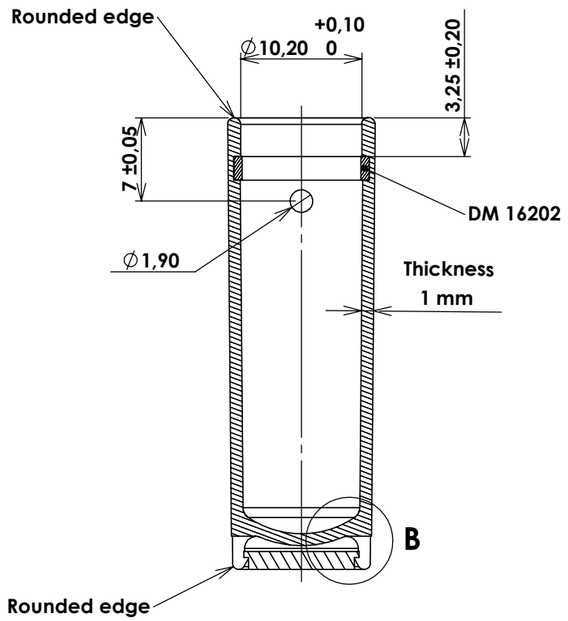
Date : 21/06/2004

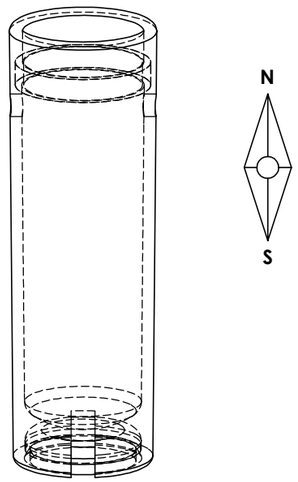
Echelle : 4:1

EMBL
Antenne de Grenoble
Laboratoire Européen de Biologie Moléculaire
6, rue Jules Horowitz - 38000 Grenoble
téléphone 0 476 207 188 - fax 0 476 207 199



COUPE A-A

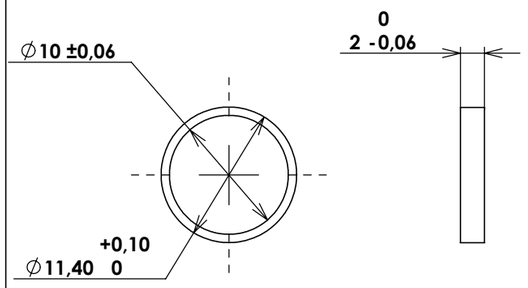




RING MAGNET POLARITY

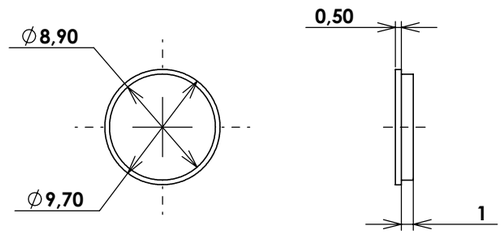
N

S



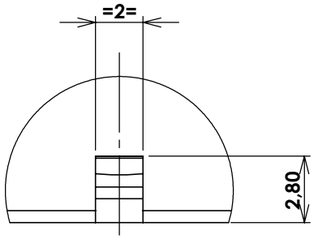
DM 16202 - Magnetic ring

Non critical dimensions

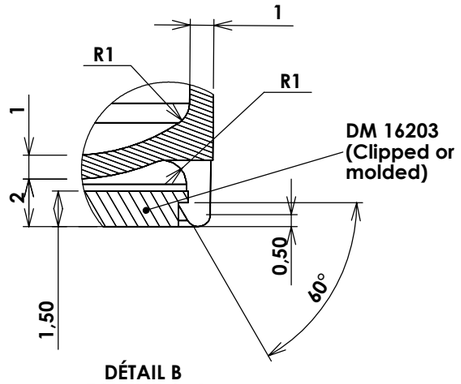


DM 12203 - Stainless ballast
Ferro-magnetic stainless steel
or Zinc plated steel

Non critical dimensions



DÉTAIL C
ECHELLE 4 : 1



DÉTAIL B
ECHELLE 4 : 1

DRAWING ONLY
FOR INFORMATION

c			
b			
a	18/06/04	Magnet polarity added	PYL
	Date	Modification	Auteur

Titre

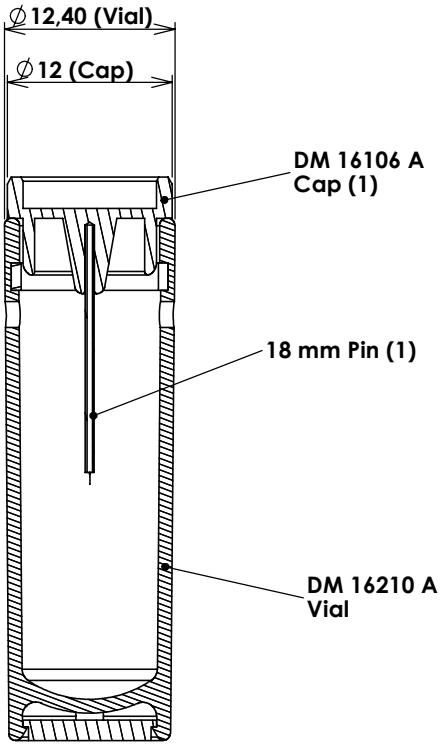
Spine Vial

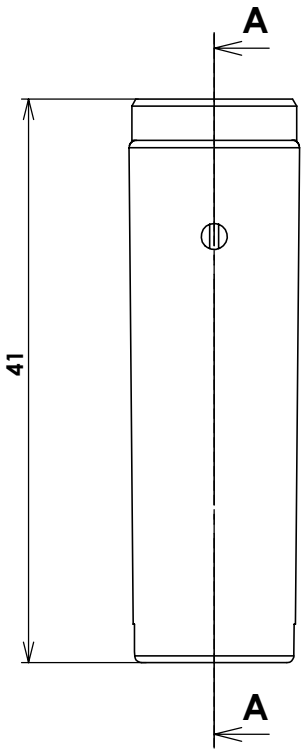
A3

Tolérances générales (sauf indications) JS13 - Ra 3,2 - angles cassés à 0,2mm

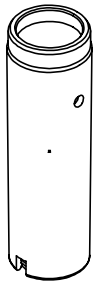
Numéro - Indice de mise à jour **DM 16210 A**	Projet : SPINE - WP6	
	Sous-ensemble :	
Matière : -	Remarque :	Qté : -
Dessiné : PY LANQUETIN	Date : 12/09/2003	Echelle : 2:1

EMBL
Antenne de Grenoble
Laboratoire Européen de Biologie Moléculaire
6, rue Jules Horowitz - 38000 Grenoble
téléphone 0 476 207 188 - fax 0 476 207 199





COUPE A-A



Drawing only for information

Note (1) : Example for HAMPTON (TM) 18 mm Pin

c			
b			
a			
	Date	Modification	Auteur

Titre

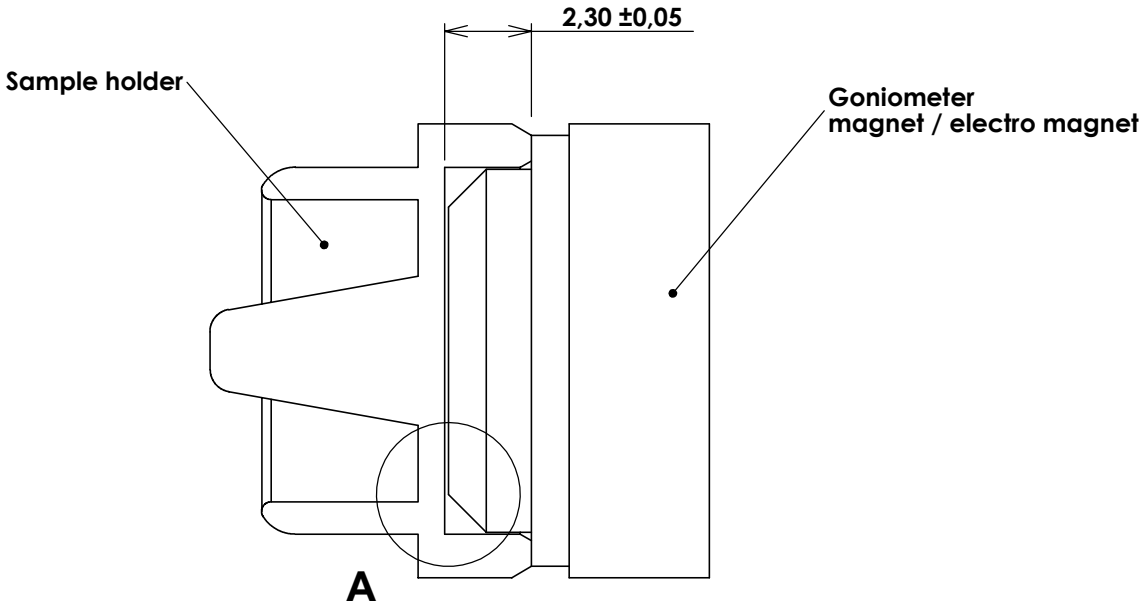
Spine sample holder + Vial

A4

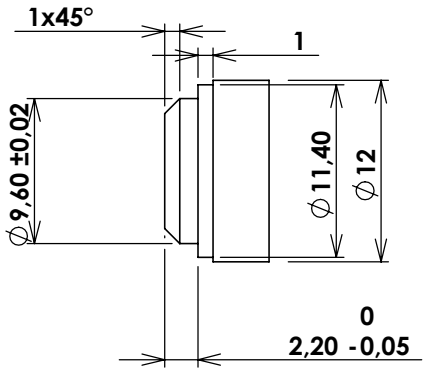
Tolérances générales (sauf indications) JS13 - Ra 3,2 - angles cassés à 0,2mm

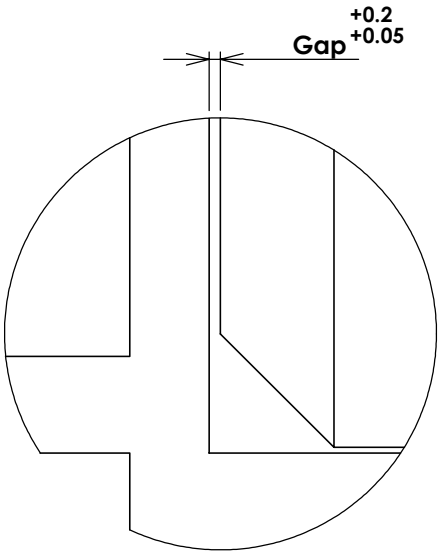
Numéro - Indice de mise à jour **DM 16001 A**	Projet : SPINE - WP6	
	Sous-ensemble :	
Matière : -	Remarque :	Qté : -
Dessiné : F. FELISAZ	Date : 30/04/2004	Echelle : 2:1

EMBL
Antenne de Grenoble
Laboratoire Européen de Biologie Moléculaire
6, rue Jules Horowitz - 38000 Grenoble
téléphone 0 476 207 188 - fax 0 476 207 199



Recommended dimensions for goniometer mount





DÉTAIL A
ECHELLE 15 : 1

c			
b			
a			
	Date	Modification	Auteur

Titre

Goniometer mount

A4

Tolérances générales (sauf indications) JS13 - Ra 3,2 - angles cassés à 0,2mm

Numéro - Indice de mise à jour **DM 16300**	Projet : SPINE - WP6	
	Sous-ensemble :	
Matière :	Remarque :	Qté : 1
Dessiné : PY LANQUETIN	Date : 23/06/2004	Echelle : 5:1

EMBL
Antenne de Grenoble
Laboratoire Européen de Biologie Moléculaire
6, rue Jules Horowitz - 38000 Grenoble
téléphone 0 476 207 188 - fax 0 476 207 199